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**Development of Generalized Pressure  
Velocity Coupling Scheme for the Analysis  
of Compressible and Incompressible  
Combusting Flows**

Contract No. NAG8-128

Progress Report

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# 1 Introduction

In the previous progress reports under the current NASA grant NAG8-128, a non-iterative pressure-velocity coupling procedure for the solution of the implicitly discretized time-dependent flow equations was described. The method was formulated for both laminar and turbulent ( $k - \epsilon$  model) flows, both incompressible and compressible. The non-iterative solutions are obtained at each time-step through a predictor-corrector sequence by the operator-splitting technique. For the last half-year, the pressure-velocity procedure has been extended to compute chemical reacting flows. In reacting flows, very large density gradients arise, leading to strong non-linear coupling of the equations. The incorporation of the species and energy equations demands significant restructuring of the predictor and corrector steps in the algorithm. These new developments will be described in this report.

# 2 Governing Equations

The governing equations for multiple species undergoing chemical reactions are the continuity, momentum, energy, and species equations. In generalized tensor notation they can be written:

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \mu \frac{\partial u_k}{\partial x_k} \right] \quad (2)$$

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_j}(\rho u_j h) = \frac{\partial}{\partial x_j} \left[ \Gamma \frac{\partial h}{\partial x_j} \right] + \sum_{i=1}^N \dot{R}_i h_{if} + \frac{\partial p}{\partial t} \quad (3)$$

$$\frac{\partial}{\partial t}(\rho f_i) + \frac{\partial}{\partial x_j}(\rho u_j f_i) = \dot{R}_i + \frac{\partial}{\partial x_j} \left( \Gamma \frac{\partial f_i}{\partial x_j} \right), \quad i = 1, 2, \dots, N \quad (4)$$

where  $\rho$  is the density;  $u_i$  the velocity;  $p$ , the pressure;  $\mu$  the effective viscosity;  $h$  the static enthalpy;  $\Gamma$  the effective diffusion coefficient;  $f_i$ , the mass fraction of chemical species; and  $\dot{R}_i$ , the chemical source term.

In addition to the equations described above, expressions are required for the thermodynamic quantities. In the present study, the JANNAF data bank and the CEC76 program were incorporated for chemical equilibrium and thermodynamic property estimations. In the CEC76 program, the minimization of the Gibbs free energy method was used to calculate the composition of chemical equilibrium species. The static enthalpy and the fluid density are then obtained by:

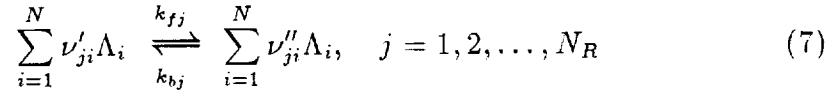
$$h = \sum_{i=1}^N f_i h_i(T) \quad (5)$$

and

$$\rho = p/R_o T \sum_{i=1}^N \frac{f_i}{Mw_i} \quad (6)$$

where  $R_o$  is the universal gas constant; and  $Mw_i$ , the molecular weight of species.

For finite rate chemistry, the gaseous  $H_2$ /Air two-step global model was used to test the proposed method. The production rates for each of the species ( $R_i$ ) required in Eq. (4) are obtained using the laws of mass action. For a general homogeneous chemical reaction, which may proceed in both the forward and reverse directions, the stoichiometric equation can be written as



where  $N_R$  is the number of reaction steps.

The law of mass continuity states that for net production of species  $i$  by reaction  $j$  is:

$$\left( \frac{dC_i}{dt} \right)_j = (\nu''_{ij} - \nu'_{ij}) \left[ k_{fj} \prod_{ij} C_i^{\nu'_{ij}} - k_{bj} \prod_{i=1}^N C_i^{\nu''_{ij}} \right] \quad (8)$$

where  $C_i$  is the concentration of species. The net rate of change in concentration of species  $i$  by all reactions is found by summing the contribution from each reaction given

$$\left( \frac{dC_i}{dt} \right) = \sum_{j=1}^{N_R} \left( \frac{dC_i}{dt} \right)_j \quad (9)$$

### 3 Solution Method

In reacting flows, a coupled implicit solution procedure of chemical kinetics/fluid dynamics problem would require the inversion of a complex system of matrices. In the present methodology, the chemical kinetics and the fluid dynamic solutions are uncoupled in performing the integration by using the operator-splitting technique. This procedure is embedded in the previously described predictor-corrector sequence with special treat on the species equation. Using the operator representation, let the governing equations be written in the following form:

$$\frac{\partial \rho f_i}{\partial t} + C(f_i) + D(f_i) = \dot{R}_i \quad (10)$$

where  $C()$  and  $D()$  are convective and diffusive operators for species  $f_i$  respectively.

To facilitate the splitting technique, the chemical kinetic solution only involves time dependent term during the predictor step. Thus, the equation

$$\frac{d}{dt} \rho f_i = \dot{R}_i(f_1, f_2, \dots, f_n) \quad (11)$$

is integrated in a fully implicit fashion. The effective chemical source terms are then determined by dividing the increment of the chemical species by the fluid residence time.

Following this, the convection and the diffusion part of the species equations are then implicitly integrated in the correction step. The corrector step integrates the fluid dynamic part with the effective chemical source terms from the predictor step as follows:

$$C(F_i) + D(f_i) = \left( \frac{d \rho f_i}{dt} \right)_{eff} \quad (12)$$

### 4 Validations

A careful validation of the present MAST code with both equilibrium chemistry and finite rate chemistry have been carried out. First, an equilibrium chemistry example involving a hypersonic viscous flow, with free stream

Mach number of 10.0 past a two-dimensional blunt body with spherical nose is tested. The Reynolds number is 8,600 and the free stream temperature is assumed to be 300 K. Figure 1 illustrates the iso-Mach contours of both the ideal gas case and the equilibrium air case. In Figure 2, calculated static temperature are plotted along the symmetric line. The effects of equilibrium chemistry on static temperature jump and shock location are significant in these calculations which agree well with other calculations in the literature.

The second case was the low-speed Burke-Schuman axi-symmetric diffusion flame. The geometry and inlet conditions are illustrated in Figure 3. The calculated flame temperature contour and mass fractions along the centerline are shown in Figure 4 and 5. The results compare very well with the analytical solutions.

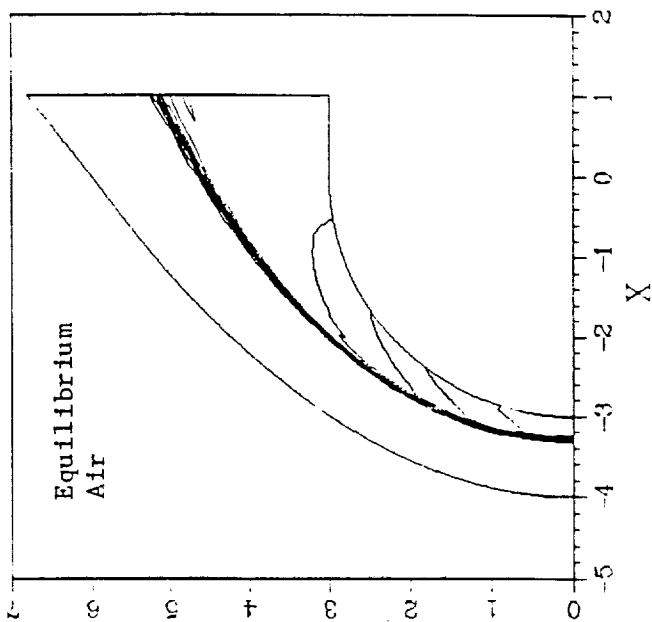
The third case was the high-speed two-dimensional wall jet flame case. The geometry and inlet conditions are illustrated in Figure 6. In this case, a sonic jet of hydrogen was injected tangentially into a Mach 2.44 vitiated airstream in a near-parallel wall. The calculated chemical composition profiles at 35.6 cm using the 2-reaction model is shown in Figure 7. Figure 8 shows the calculated static temperature profile at  $x = 35.6$  cm. These results compare well with the experimental data.

The fourth case involves a cold hydrogen ( $T = 251K$ ) of Mach 2.0 injected along the axis of a circular supersonic stream of hot vitiated air ( $T_\infty = 1485K$ ) as shown in Figure 9. Figure 10 shows predictions of  $H_2$ ,  $O_2$ , and  $H_2O$  mass fractions at  $x/d_j = 27.9$ . Figure 11 shows temperature contours for this configuration.

## 5 Summary and Plans

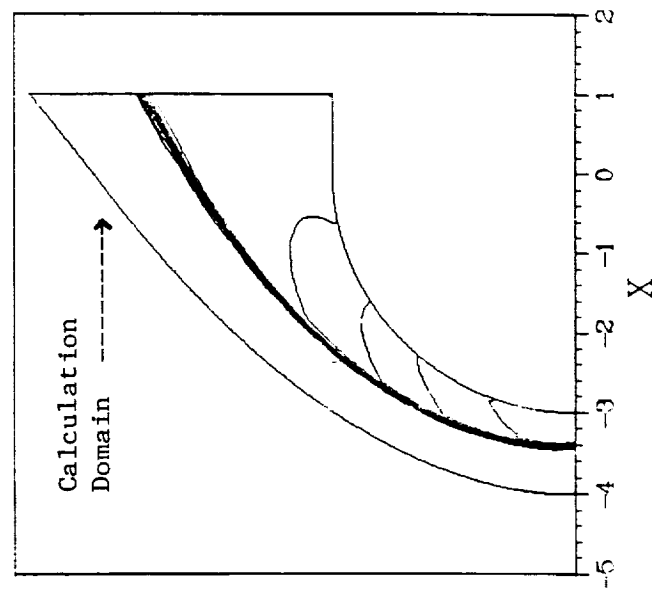
The operator-splitting method involving chemical reaction for both equilibrium chemistry and finite rate chemistry has been successfully developed and implemented into the new pressure-velocity coupling scheme for chemical reaction flow calculations. This next year's plan is to combine the two-phase (Eulerian-Lagrangian) aspect into the pressure-velocity coupling procedure for full spray-combustion calculations.

CONTOUR OF MACH NUMBER [M=10., 81\*41]



(a)

CONTOUR OF MACH NUMBER [M=10., 81\*41]



(b)

Figure 1. (a) Ideal Gas (Air), (b) Real Gas (Equilibrium Chemistry)

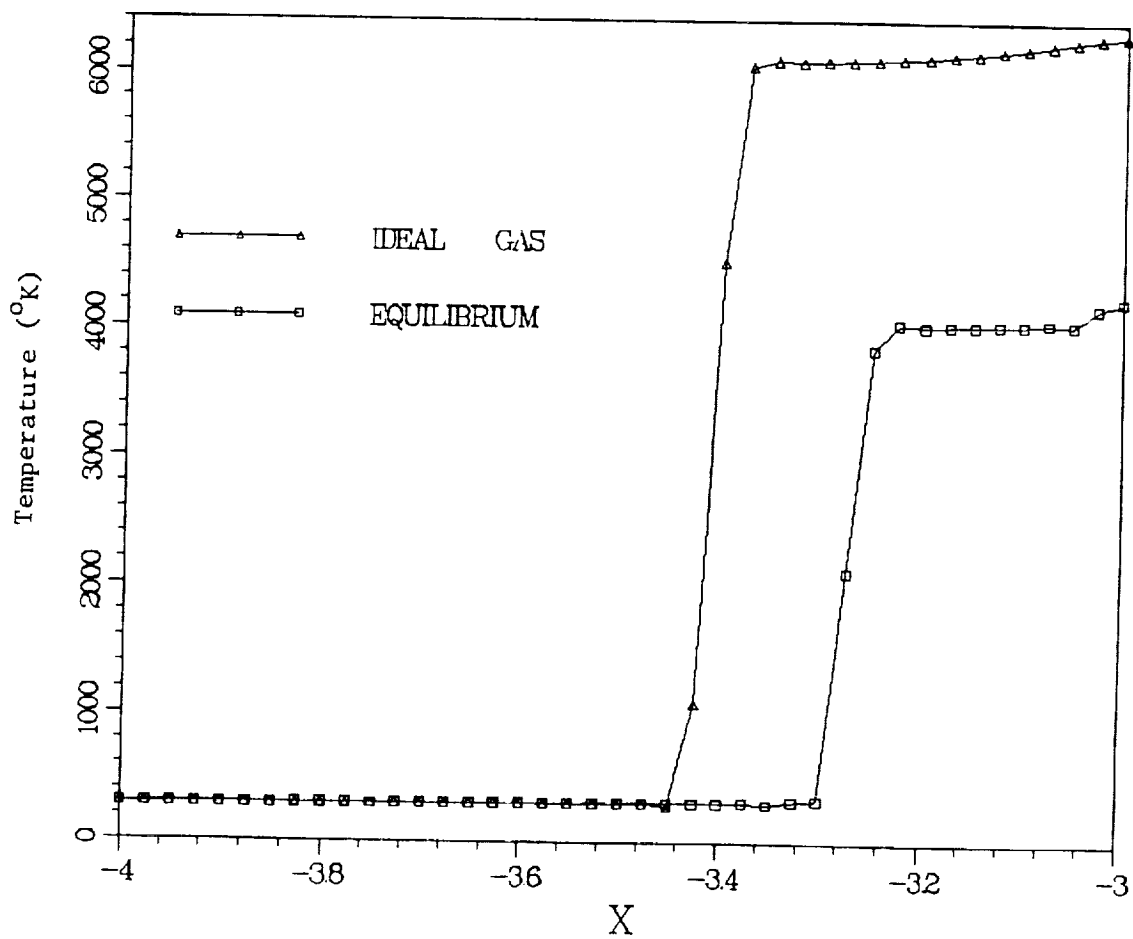


Figure 2. Temperature Along Symmetric Line

BURKE - SCHUMANN DIFFUSION FLAME

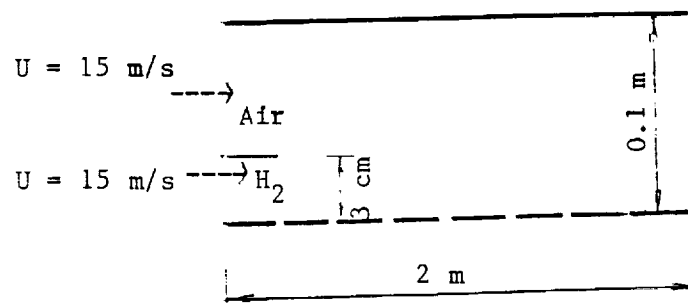


Figure 3. Burke - Schumann Diffusion Flame



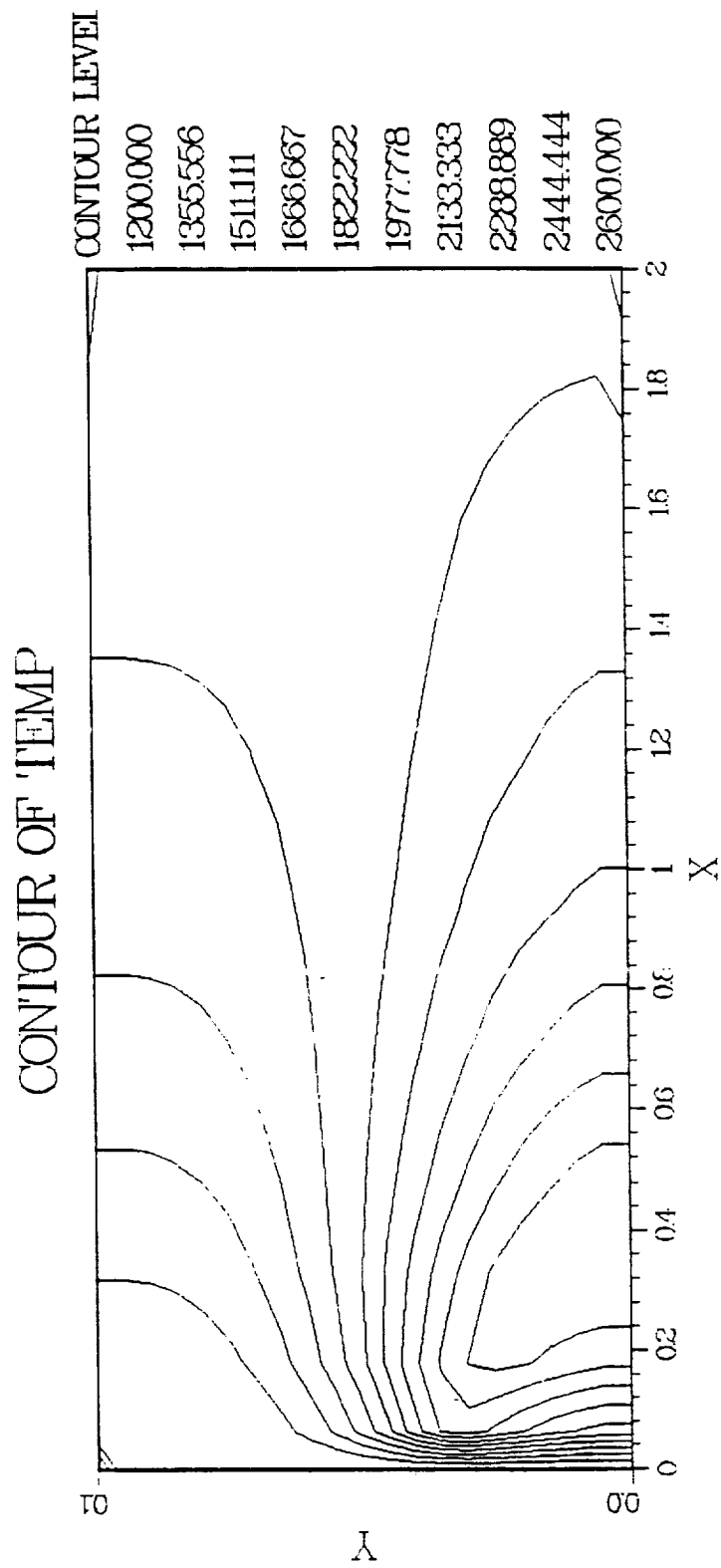


Figure 4. Temperature Contours of the Burke-Schumann Diffusion Flame

# BURKE SCHUMANN DIFFUSION FLAME

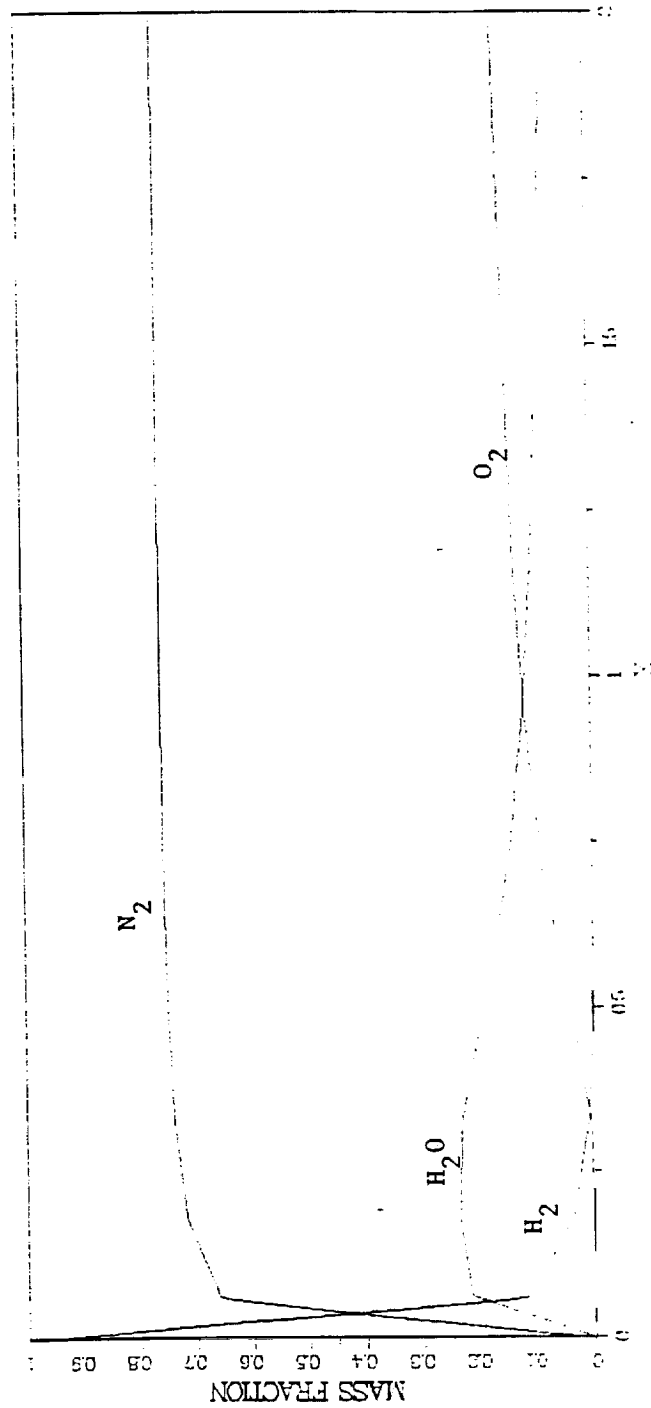
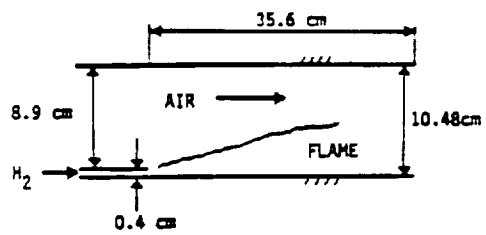


Figure 5. Mass Fraction Along the Centerline of the Diffusion Flame



	H2 Jet	Main Stream
M	1.0	2.44
T, (K)	254	1270
U, (m/s)	1216	1764
P, (Mpa)	0.1	0.1

Figure 6. Two-dimensional case by Burrow & Kurkov

# TWO-DIMENSIONAL FLOW WITH FUEL INJECTIONS

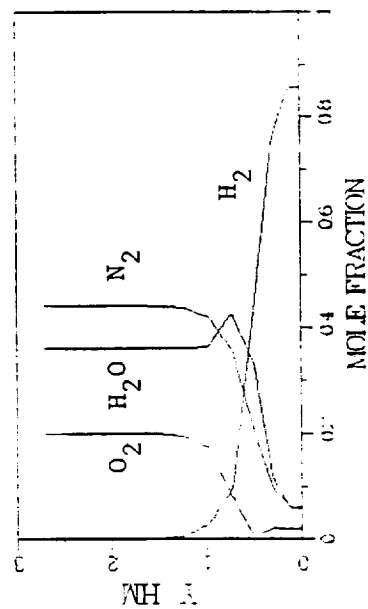


Figure 7. Mass Fraction Profiles at 35.6 cm

TWO-DIMENSIONAL FLOW WITH FUEL INJECTIONS

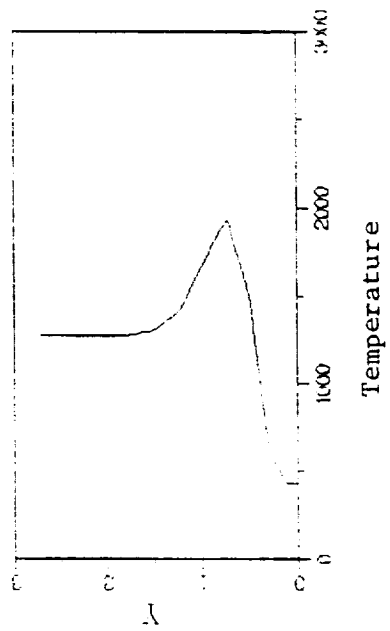


Figure 8. Temperature Profile at 35.6 cm

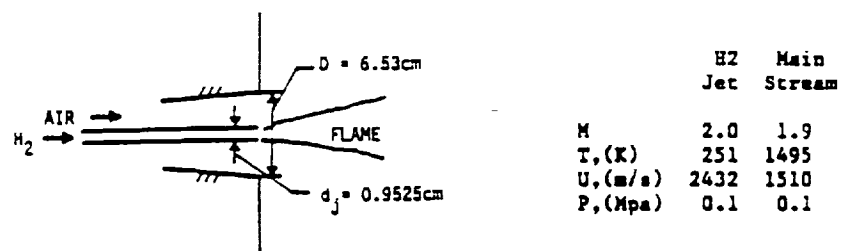


Figure 9. Axisymmetric Case by Henry & Beach

# TWO-DIMENSIONAL JET WITH FUEL INJECTIONS

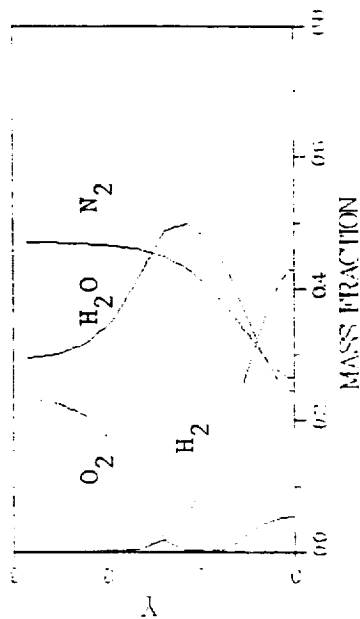


Figure 10. Mass Fraction Profiles at  $\frac{x}{d_i} = 27.9$

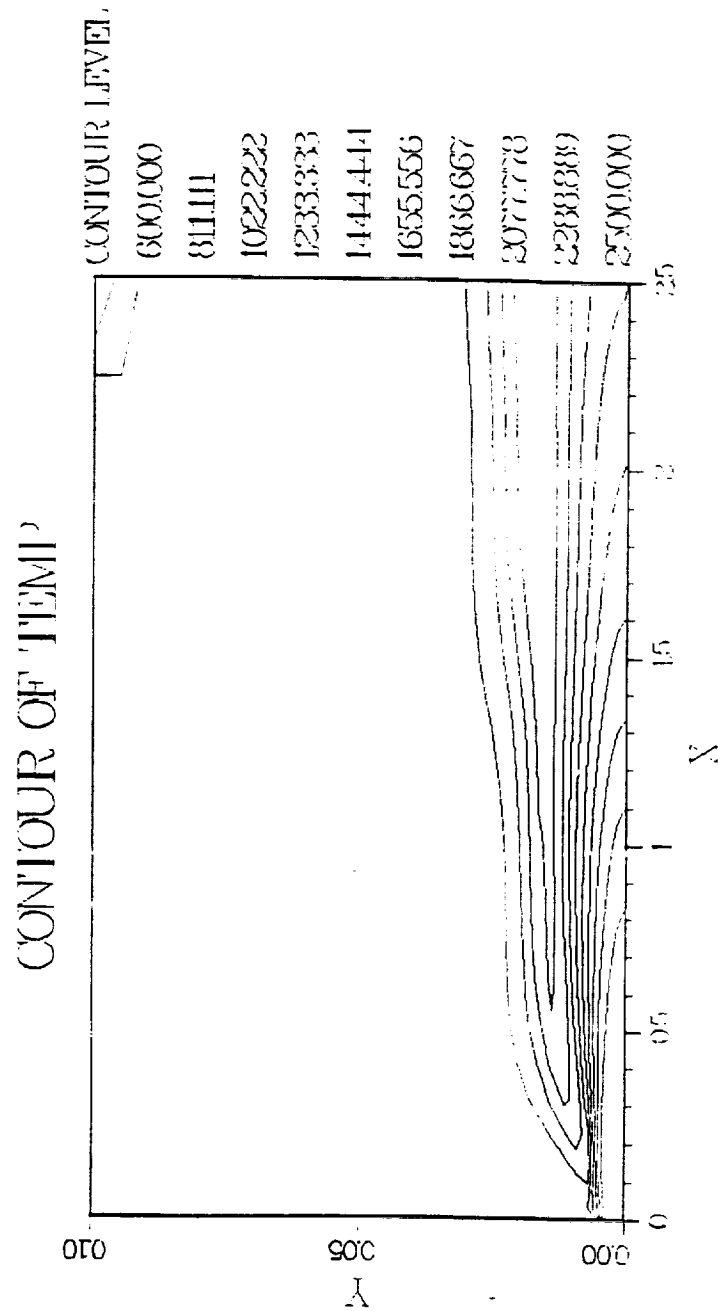


Figure 11. Temperature Contours